PB86-103660

Atmospheric Diffusion Modeling Based on Boundary Layer Parameterization

(U.S.) Environmental Protection Agency
Research Triangle Park, NC

Sep 85

U.S. Department of Commerce
National Technical Information Service
NTIS

PB86-103660

EPA/600/3-85/056
September 1985

ATMOSPHERIC DIFFUSION MODELING BASED ON BOUNDARY LAYER PARAMETERIZATION

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TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
EPA/600/3-85/056		PB86 103607AS

4. TITLE AND SUBTITLE	5. REPORT DATE
ATMOSPHERIC DIFFUSION MODELING BASED ON BOUNDARY LAYER PARAMETERIZATION	September 1985
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) J.S. Irwin[1], S.E. Gryning[2], A.A.M. Holtslag[3], B. Siversten[4]	8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS 1. ASRL, RTP, NC, USA 2. Risø National Laboratory, Roskilde, DENMARK 3. KNMI, DeBilt, THE NETHERLANDS 4. LILU, Lillestrøm, NORWAY	10. PROGRAM ELEMENT NO. CDTA1D/08 - 2182(FY85)
	11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS Atmospheric Sciences Research Laboratory - RTP, NC Office of Research and Development U. S. Environmental Protection Agency Research Triangle Park, NC 27711	13. TYPE OF REPORT AND PERIOD COVERED Final
	14. SPONSORING AGENCY CODE EPA/600/09

15. SUPPLEMENTARY NOTES

16. ABSTRACT

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17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS (This Report)	21. NO. OF PAGES
RELEASE TO PUBLIC	UNCLASSIFIED	54
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE A11.95

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

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The information in this document has been funded in part by the United States Environmental Protection Agency (EPA), under agreement DW-13931239 between the EPA and the Air Resources Laboratories (ARL), National Oceanic and Atmospheric Administration (NOAA). It has been subjected to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Approval does not signify that mention of trade names or commercial products constitute endorsement or recommendation for use.

AFFILIATION

Mr. John S. Irwin is on assignment from the National Oceanic and Atmospheric Administration, U. S. Department of Commerce.

PREFACE

During September 12-16, 1983 at the Royal Netherlands Meteorological Institute and in June 25-29, 1984 at the Risø National Laboratory, a workgroup of scientists from four air research and meteorological agencies met to review and discuss methods for characterizing diffusion meteorology. The contents of this report summarizes the discussions of these meetings. Based on this report, the workgroup drafted two papers which were presented at the 15-th International Technical Conference on Air Pollution Modeling and Its Application (16-19 April 1985 at St. Louis, MO):

Parameterization of the atmospheric boundary layer for air pollution diffusion models by A.A.M. Holtslag, S.E. Gryning, J.S. Irwin and B. Sivertsen.

Atmospheric dispersion modeling based upon boundary layer parameterization by B. Sivertsen, S.E. Gryning, J.S. Irwin and A.A.M. Holtslag.

These two papers extend the concepts presented in this report and demonstrate the performance of the suggested dispersion modeling using nonbuoyant tracer data from field experiments conducted in Denmark and Norway. A bound version of the proceedings of the conference will be made available through Plenum Press as Air Pollution Modeling and Its Application V.

ABSTRACT

The conclusions of a workgroup are presented outlining methods for processing meteorological data for use in air quality diffusion modeling. To incorporate the proper scaling parameters the discussion is structured in accordance with the current concepts for the idealized states of the planetary boundary layer. We recommend a number of models, the choice of which depends on the actual idealized state of the atmosphere. Several of the models characterize directly the crosswind integrated concentration at the surface, thus avoiding whenever justified the assumption of a Gaussian distribution of material in the vertical. The goal was to characterize the meteorological conditions affecting the diffusion for transport distances on the order of 10 km or less. Procedures are suggested for estimating the fundamental scaling parameters. For obtaining the meteorological data needed for estimating the scaling parameters, a minimum measurement program to be carried out at a mast is recommended. If only synoptic data are available, methods are presented for the determination of the scaling parameters. Also, methods are suggested for estimating the vertical profiles of wind velocity, temperature, and the variances of the vertical and lateral wind velocity fluctuations.

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LIST OF SYMBOLS

a = an empirical constant, used in Eq (4-4) in the estimation of the nighttime potential temperature profile

a_1, a_2 = empirical constants used in shape parameter equations
b_1, b_2
c, p

b = empirical constant, used in Eq (5-15)

A, B = shape constant functions used to describe general solution to the two-dimensional diffusion equation

A_w = empirical constant, used in Eq (4-5) in the estimation of the variance of the vertical wind speed fluctuations

d, d_1, d_2 = empirical constants used in parameterization of the net radiation
c, c_1, c_2
c_3

c_4, c_5 = empirical constant, used to determine mixing height in Eq (3-7)

c_6 = empirical constant, used to determine mixing height in Eq (3-8)

c_p = specific heat capacity at constant pressure

d = empirical constant, used in Eq (4-5) in the estimation of the variance of the vertical wind speed fluctuations

D = angle between the surface wind direction and the geostrophic wind direction

f = Coriolis parameter

f_s, f_g = weighting functions used in the estimation of the vertical profile of the wind

f_y, f_z = empirical functions describing the growth of the disperision parameters, σ_y and σ_z

F = plume buoyancy, $gQ_H/\pi\rho c_p T_o$

F^* = plume buoyancy parameter, $F/(Uw_*^2 z_i)$

g = acceleration due to gravity

G = geostrophic wind speed

G_o = soil heat flux

h = surface temperature inversion height

$H = \rho c_p \overline{w'\theta'}$, sensible heat flux

H_I = integral of heat flux, Eq (4-4)

k = Von Karman constant

K = vertical eddy diffusivity of matter

L = Monin-Obukhov length

N = fraction of sky covered by cloud

N = Brunt-Vaisala frequency

$p_s = F/(U\gamma_i z_i'^3)$

P = fraction of material that stabilzes in capping inversion

Q = emission rate

Q_H = rate of output of heat from a chimney

Q^* = net radiation

r = albedo of surface

R_o = Rossby number

$R(\xi)$ = Lagrangian autocorrelation function

s = shape parameter, Eq 5-13 and Eq 5-14

t_o = transition time, the instant when the net sensible heat flux at the surface changes sign from positive to negative

T = air temperature

T_e = empirical time scale, used in Eq (5-5)

T_L = Lagrangian integral time scale

T_o = stack gas temperature

u = horizontal wind speed

u_f = free convection scaling velocity

u_* = $\sqrt{\tau/\rho}$ surface friction velocity

U = estimated horizontal wind speed assuming surface layer similarity

U_r = near-surface reference wind speed

U_z, V_z = components of horizontal wind in the vertical relative to a coordinate system alined along the surface-layer reference wind direction

w_* = mixed layer scaling velocity

x,y,z = rectangular coordinates, x usually along mean wind and z vertical

x_o = integration constant used in describing variation of the mean height of particles as a function of distance downwind

x' = typical distance to upwind obstacle

X = $(x/z_i)(w_*/U)$

X' = $(x/z_s)(w_*/U)$

z_o = surface roughness length

z_r = measurement height of the near-surface reference wind speed

z_s = release height above ground

z_i = mixing height

α = empirical constant, accounts for the strong correlation between surface heat flux, net radiation and soil heat flux in Eq (3-2)

β = empirical constant, accounts the portion of the sensible heat flux not related to the net radiation or the soil heat flux in Eq (3-2)

γ_i = lapse rate above unstable mixed layer

γ/s = thermo-dynamic function of temperature

ΔT = vertical temperature difference

$\Delta\theta$ = used in defining the nighttime potential temperature profile, $\theta(t,z)-\theta_o$

$\Delta\theta_i$ = potential temperature jump at top of unstable mixed layer

$\Delta\theta_s = \theta_s(t) - \theta_o$

$\zeta = z/L$

$\zeta_r = z_r/L$

θ = potential temperature

θ_{BL} = mixed layer temperature

$\theta(t,z)$ = nighttime potential temperature

$\partial\theta/\partial z$ = potential temperature gradient

θ_f = free convection scaling temperature

θ_m^* = mixed layer scaling temperature

θ_o = the potential temperature of the adiabatic profile at transition time

$\theta_s(t)$ = the surface potential temperature found at time t since transition

θ^* = surface layer scaling temperature

κ = horizontal wave number

ℓ = the length scale, estimated as, $(1/\ell_s + 1/\ell_n)^{-1}$ where ℓ_s is the stable length scale and ℓ_n is the neutral length scale,

$\ell_s = \gamma^2 \sigma_w/N$, where $\gamma = 0.522$,

$\ell_n = \alpha z$, where $\alpha = 0.36$,

Λ = local Monin-Obukhov length

ξ = height of major obstacles over relatively smooth terrain

ρ = air density

σ_u = standard deviation of the horizontal wind speed deviations

σ_v = standard deviation of the crosswind speed diviations

σ_w = standard deviation of the vertical wind speed deviations

σ_y = root mean squared deviation of the cross-wind concentration distribution

σ_z = root mean squared deviation of the vertical concentration distribution

σ_{yb} = induced lateral dispersion due to buoyancy effects

σ_{yo} = lateral dispersion due to ambient turbulence

σ_{ys} = induced lateral dispersion due to wind direction shear in the vertical

σ_{zo} = vertical dispersion due to ambient turbulence

σ_{zb} = vertical dispersion due to buoyancy effects

τ = $-\rho\overline{u'w'}$, momentum shear stress

ϕ = elevation of sun above horizon

$\phi_h(z/L)$ = dimensionless empirical function in the surface layer, $(kz/\theta)\partial\theta/\partial z$

$\phi_m(z/L)$ = dimensionless empirical function in the surface layer, $(kz/u_*)\partial u/\partial z$

$\chi(x,y)$ = surface concentration

χ^y = crosswind integrated concentration

Ψ = stability dependent terms of the wind speed profile

1. INTRODUCTION

The purpose of the following discussion is to outline a set of methods for processing meteorological data for use in diffusion modeling. In this discussion, the emphasis will be on those methods considered both physically realistic and numerically efficient.

Most of the early attempts to estimate the diffusion of air pollutants were based on the Gaussian-plume model, for example see Sutton (1953). Pasquill (1961) gave simple rules for obtaining the lateral spread based on wind-direction trace data and suggested the effects of thermal stratification in the lower atmosphere be represented in broad categories of stability, defined in terms of meteorological data routinely available in surface weather observations. By the early 1970's, air quality simulation models were viewed as a means to estimate the relative magnitudes of concentration distributions from various sources and thereby provide a rational basis for strategies leading to air quality improvement or maintenance. Most of the air quality simulation models developed in response to these modeling requirements were based on the general Gaussian-plume model. Invariably the models were constructed assuming that the dispersive characteristics of the atmosphere were vertically and horizontally homogeneous.

Current concepts regarding the structure of an idealized boundary layer, are briefly reviewed and the basic meteorological variables of interest to diffusion modeling are identified. Methods are proposed for specifying each of these basic variables. The goal is to characterize the meteorological

conditions affecting the diffusion for transport distances on the order of 10 km or less over reasonably flat and homogeneous terrain. In this description of turbulence, the effects of clouds and fog are only considered as far as these affect the radiation and the surface energy balance. The relationship and importance of the variables to diffusion processes are reviewed. The final section reviews the conclusions and envisioned future research activities.

2. THE BOUNDARY LAYER

Atmospheric diffusion is controlled by the turbulence in the air. The parameters describing the scales of turbulence are therefore of fundamental importance in a description of atmospheric diffusion. Most air pollution sources emit into the boundary layer which can be defined as the lower layer of the atmosphere where the influence of the surface is present due to friction. The character and turbulent state of the boundary layer is strongly affected by the diurnal heating and cooling cycle.

2.1 The Unstable Boundary Layer

The unstable boundary layer is directly affected by solar heating of the ground. The layer has a very pronounced diurnal variation, and typically reaches a height of 1-2 km over land in summertime. For the characterization of turbulence within this layer three length scales are important. These are the mixing height, z_i, the height above the ground, z, and the Monin-Obukhov stability length, L. The mixing height z_i defines the height above the surface in which pollutants are mixed by presence of turbulence. From these three parameters, two independent dimensionless parameters can be formed. The unstable boundary layer can be divided into several layers defined in terms of these parameters. Fig. 2-1 is a schematic diagram showing idealized limits of validity of the scaling techniques together with the corresponding parameters for the turbulence. This figure is similar to those presented by Nicholls and Readings (1979) and Olesen et al. (1984). Traditionally, the boundaries between the individual layers have not been expressed in the same set of dimensionless parameters. This makes any sketch of the boxes look

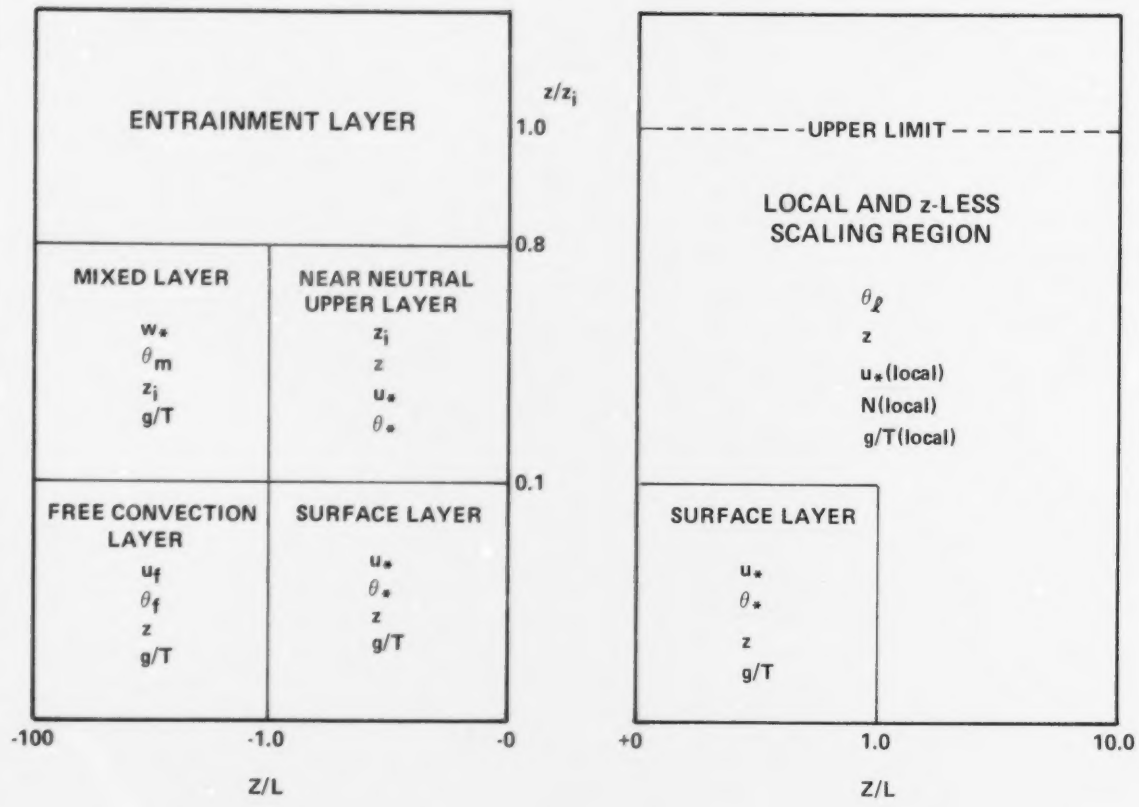

Figure 2-1. Idealized view of the states of the Planetary Boundary Layer and the limits of validity of the scaling techniques.

fairly complicated. Here, we have sacrificed some of the detailed structure that arises from the traditional way of describing the boundaries. Our proposed simplified version in some cases slightly deviates from the viewpoints traditionaly held of the boundaries.

2.1.1 The surface layer ($z_o \ll z$, $\text{Min}(0.1z_i;-L)$)

This is the layer where wind shear plays a dominant role. The controlling parameters are the height, z, the momentum shear stress, $\tau = -\rho\overline{u'w'}$, the sensible heat flux at the ground, $H = \rho c_p\overline{w'\theta'}$, and the buoyancy parameter, g/T (Businger, 1973). From these parameters we can form the equivalent parameters, z, L, u_* and θ^* where L is the Monin-Obukhov length, $L = -u_*^3/[k(g/T)(H/\rho c_p)]$, k the Von Karman constant (~0.4), the friction velocity $u_* = \sqrt{\tau/\rho}$ and the scaling temperature $\theta^* = -H/(\rho c_p u_*)$. Monin-Obukhov similarity theory postulates that dimensionless local groups formed with u_* and θ^* become universal functions of z/L. The surface layer is confined to the layer $20z_o < z < -L$ and $z < 0.1z_i$, where z_o is the surface roughness length.

2.1.2 The free convection layer ($-L < z < 0.1z_i$)

Above z = -L, is a layer where τ is no longer important in describing the atmospheric turbulence and z_i is not yet important, thus the controlling parameters are z and the surface layer values of $\overline{w'\theta'}$ and g/T. The free convection layer exists for $-L < z < 0.1z_i$. Tennekes (1970) described the scaling velocity and temperature as,

$$u_f = (\overline{w'\theta'}\ z\ g/T)^{1/3},$$

$$\theta_f = \overline{w'\theta'}/u_f.$$

2.1.3 The mixed layer ($0.1z_i < z < 0.8z_i$ and $z/-L > 1$)

In this layer the turbulence structure is insensitive to τ as in the free convection layer, but also the height loses its importance as a scaling parameter. Hence the mixing height, z_i, emerges as the controlling length scale. The scaling velocity and temperature become, Deardorff (1970),

$$w_* = (z_i \; g/T \; \overline{w'\theta'})^{1/3},$$

$$\theta_m = \overline{w'\theta'_s}/w_*,$$

where $\overline{w'\theta'}$ and g/T are surface layer values.

2.1.4 The entrainment layer ($0.8z_i < z < 1.2z_i$)

The turbulence structure is dominated by entrainment processes from the overlying stable air in the capping inversion. The turbulence structure in this region is poorly understood. Recent measurements suggest that the distance to the inversion, $|z_i - z|$ enters as a scaling length, see Driedonks and Tennekes (1984). The scaling velocity and temperature relevant to this layer have not as yet been proposed.

2.1.5 Near neutral upper layer ($0.1z_i < z < 0.8z_i$ and $z/|L| < 1$)

The layer will only rarely be found over land but is not unusual over the sea. The scaling parameters for the surface layer are relevant for the near neutral upper layer; in addition the height of the inversion, z_i, is also important. For profiles of mean quantities the Rossby number, $R_o = G/fz_o$ (G the geostrophic wind speed and f the Coriolis parameter) might be of importance.

2.2 The Stable Boundary Layer

The stable boundary layer is created by cooling of the air adjacent to the ground. The depth of the inversion layer, h, is often taken as the height at which the (negative) heat flux has fallen to a certain (low) proportion of its surface value. The study of the stable boundary layer is much less advanced than its unstable counterpart. As buoyancy forces suppress the turbulence under stable conditions, the magnitude of fluctuations generally are very low and consequently difficult to measure. Also the structure of the turbulence is masked by other physical processes that are supported in a stable atmosphere. Such processes are gravity waves, drainage and slope flows, intermittent turbulence and radiation divergence. The coexistence of these processes and turbulence complicate the interpretation of the data. No simple relation exists between the depth of the surface inversion, h, and the mixing height, z_i, through which the turbulence exchange processes take place. The depth, z_i, of the turbulent stable boundary layer can become progressively smaller at the same time as the depth of the surface based inversion h grows.

2.2.1 The surface layer ($z_o \ll z$, Min $(0.1z_i; L)$)

This layer is the stable counterpart of the unstable surface boundary layer, and the same scaling parameters apply. The layer is in principle lower than the height, $z \simeq L$ or $z < 0.1\ z_i$, whichever is smaller. Most times the limit is given by $0.1z_i$.

2.2.2 Local and z-less scaling region ($\mathrm{Min}(0.1z_i;L) < z < z_i$ and $z/L < 10$)

The range where local scaling applies is still unsettled and a matter of discussion. We define it as the whole stable boundary layer except the surface layer part. The local scaling approach is an extension of Monin-Obukhov similarity theory to the whole stable boundary layer (Nieuwstadt, 1984). Here Λ is called the local Monin-Obukhov length, defined as $\Lambda = -u_*^3/[k(g/T)\overline{w'\theta'}]$ where u_* and $\overline{-w'\theta'}$ are the local values of the kinematic momentum flux and heat flux. The temperature scale for this region can be defined as $\theta_\ell = (w'\theta')/u_*$. In the local scaling region only two length scales arise, z and Λ. Nieuwstadt's (1980b) model of the stable boundary layer suggests that $\Lambda \sim L\,(1-z/h)^{5/4}$. As $z/\Lambda \to 1$, local scaling conforms to z-less scaling (Wyngaard, 1973), where z is no longer an important length scale for the turbulence. This results from the stable temperature stratification becoming increasingly more effective in inhibiting vertical motions. The turbulence within the z-less region is intermittent and difficult to characterize. Some success has been achieved in describing the low frequency part of the horizontal velocity spectra using the local value of the Brunt-Vaisala frequency $N^2 = (g/T)(\partial\theta/\partial z)$.

3. BASIC PARAMETERS

3.1 The Surface Roughness Length

The surface roughness length z_o forms the lower boundary in diffusion models (Pasquill and Smith, 1983). The length z_o is in principle the height at which the wind speed is zero. The length z_o is related to the roughness characteristics of a homogeneous terrain or landscape. When the terrain is homogeneous, the roughness length can be determined from wind profiles observed in near-neutral conditions.

Very often, we have relatively smooth terrain disturbed by occasional obstructions or by large perturbations. In such cases an effective roughness length was found appropriate for use in the flux-profile relations (Nieuwstadt, 1978; Beljaars, 1982). As discussed by Wieringa (1981) and Beljaars (1982) for a rough to smooth transition, the turbulence adjusts more slowly to the underlying surface than does the wind profile. For this reason the roughness averaged over the upwind fetch can be better evaluated from $\sigma_u/\overline{u}$ or gustiness than from wind profiles (Wieringa, 1976, 1980). σ_u is the root mean squared (rms) variance of the wind speed u and $\overline{u}$ is the average wind speed. Conversely, this means that the wind profile can be described with the effective roughness length only above a certain height. Beljaars (1982) estimates this height as 2ξ, where ξ is the height of the major obstacles. Closer to the surface the flux-profile relations differ from those over uniform terrain (Beljaars et al., 1983) and are usually location dependent (Wieringa, 1981). When no measurements are available, we can obtain from a visual terrain description a crude value for the effective roughness length (Hogstrom and Hogstrom, 1978; Davenport, 1960). In Table

3-1 an example is given. For the application of the above methods for determining z_o, we select as many wind direction sectors as needed to distinguish between major variations. In general, no sectors less than 30 degrees in angular extent are expected to be suitable in practice.

TABLE 3-1. TERRAIN CLASSIFICATION IN TERMS OF EFFECTIVE SURFACE ROUGHNESS LENGTH z_o. TABLE PARTLY EXTRACTED FROM DAVENPORT (1960).

Short terrain description	z_o(m)
Open sea, fetch at least 5 km	0.0002
Mud flats, snow; no vegetation, no obstacles	0.005
Open flat terrain; grass, few isolated obstacles	0.03
Low crops, occasional large obstacles, $x'/\xi > 20$*	0.10
High crops, scattered obstacles, $15 < x'/\xi < 20$	0.25
Parkland, bushes, numerous obstacles, $x'/\xi \simeq 10$	0.5
Regular large obstacle coverage (suburb, forest)	(0.5 - 1.0)

* x' = typical distance to upwind obstacle; ξ = height of obstacle.

3.2 The Monin-Obukhov Length

From the surface fluxes of sensible heat and momentum, the Monin-Obukhov length for dry air can be formed,

$$L = - u_*^3/[k(g/T)(H/\rho c_p)], \qquad (3\text{-}1)$$

Here we have ignored the moisture influence which is typically small above a land surface. Values for u_*, H and thus L can be obtained from turbulence measurements.

When no turbulence measurements are available the fluxes can be obtained from profiles of wind and temperature near the surface (Businger et al., 1971; McBean, 1979; Irwin and Binkowski, 1981). The profile method gives good agreement with turbulence measurements and energy budget measurements, if an effective roughness length is used in the wind profile (Nieuwstadt, 1978). These derived fluxes are representative for a larger area than would be measured with an instrumented meteorological tower located on-site. This becomes important, for instance, for the estimation of wind profiles at larger heights from a single wind speed and the surface fluxes. In such cases, the surface fluxes should be representative of the larger area. This is demonstrated by Korrell et al. (1982) for the Boulder tower and by Beljaars (1982) and Holtslag (1984a) for the Cabauw tower. Furthermore, the horizontal velocity fluctuations scale on the friction velocity representative of the larger area (Beljaars et al., 1983).

When a vertical temperature profile in the surface layer is not available, we must parameterize the sensible heat flux H. Holtslag and Van Ulden (1983) and Van Ulden and Holtslag (1983) have given procedures for the derivation of the sensible heat flux from routine weather data.

During daytime over land, H is obtained from a modified Priestley-Taylor formula (De Bruin and Holtslag, 1982),

$$H = \frac{1 - \alpha + \gamma/s}{1 + \gamma/s} (Q^* - G_o) - \beta \ , \qquad (3\text{-}2)$$

where Q* is net radiation, G_o is soil heat flux (typically 0.1Q*). γ/s equals $c_p/(\lambda\partial q_s/\partial T)$ where λ is the latent heat of water vaporization and q_s is the saturation specific humidity. For T between -5 and 35 C, γ/s can be approximated as exp[(279.57-T)/17.78], T in degrees K. It can be shown that when saturated air passes over a wet surface $\alpha \rightarrow 1$ and $\beta \rightarrow 0$ (Priestley, 1959). For other climatological and surface conditions α and β must be adjusted. Table 3-2 shows typical values for α and β as a function of surface moisture availability. Reiff et al. (1984) use (3-2) with $\alpha = 1$ and β as a varying function of time. Around sunrise, $\beta = 0$, but β increases with time up to $\beta = 20\ Wm^{-2}$ in a few hours.

In Holtslag and Van Ulden (1983) procedures are discussed for the evaluation of Q* from the fraction of sky covered by cloud, N, the elevation of the sun above the horizon, ϕ , and the shelter temperature,

$$Q^* = \frac{(1 - r)[d_1 \sin\phi + d_2](1 + cN^d) + c_1T^6 + c_2N}{1 + c_3} \qquad (3\text{-}3)$$

where r is the albedo of the surface (typically 0.26 for short grass). Values for the empirical constants in (3-3) $[d, d_1, d_2, c, c_1, c_2]$ are $[3.4,\ 990Wm^{-2},\ -30Wm^{-2}, -0.75, 5.31x10^{-13}Wm^{-2}K^{-6}, 60Wm^{-2}]$. Values for the surface heating cofficient c_3 are listed in Table 3-2. This parameter describes the relative increase of surface temperature with net radiation Q*. As shown by Holtslag and Van Ulden c_3 depends primarily on α and air temperature T. Therefore, α is the crucial parameter for the surface energy budget parameterization (see De Bruin, 1983; Van Dop, 1983). In combination with α, β and c_3 the sensible heat flux is obtained from (3-2). Afterwards, u_* and L are obtained from (3-1) and a single wind speed observation and the

integrated wind profile. The values of α, β and c_3 should reflect the site. At present, we suggest the values listed in Table 3-2 be used for guidance.

TABLE 3-2. TYPICAL VALUES OF THE COEFFICIENTS α, β AND c_3 FOR SEVERAL CASES. NOTE THAT c_3 IS A FUNCTION OF AIR TEMPERATURE T AS WELL (SEE HOLTSLAG AND VAN ULDEN, 1983). α AND c_3 ARE DIMENSIONLESS AND β HAS THE UNITS OF Wm^{-2}.

Description	α	β	c_3	Example
Advection of saturated air above wet surface.	1	0	-	A wet surface is a water surface or a land surface covered with a thin water layer.
Advection of unsaturated air above wet surface.	1.3	0	-	A saturated surface is a water surface or a moist cropped land surface.
Advection of unsaturated air above a relatively moist surface.	1 or 1.15	20 or 0	0.12 (T=288K)	Typical Dutch surface conditions, green growing grass, no lack of water.
Relatively dry surface conditions.	0.45	9	0.25 (T=300K)	Obtained from the Prairie Grass data.
Bare soil, no vegetation, no water available.	0	0	0.38 (T=300K)	Typical values for cities, railways, highways and bare soil(no evaporation).

During nighttime the best way to estimate the sensible heat-flux and thereby the Monin-Obukhov length is from the profiles of wind and temperature as discussed at the beginning of this section.

A simple analysis indicates that a constant value of θ_* can be assumed during nighttime. The sensible heat flux can be obtained from an approximation for the scaling temperature, θ_*. A typical value for clear conditions is $\theta_* \simeq 0.1K$ (Venkatram, 1980). Van Ulden and Holtslag (1983) present methods for estimating θ_* as a function of total cloud cover.

3.3 Mixing Height And Inversion Height

The mixing height z_i defines the layer above the surface through which pollutants are mixed by the presence of turbulence. During daytime convective conditions or neutral stability conditions the mixing height may extend to the height where vertical mixing is capped by the inversion (inversion height h). During nighttime stable conditions, however, it is important to distinguish between the mixing height z_i and the surface inversion depth h. In part, the difference between z_i and h results because the turbulence is supressed in the presence of a stable temperature gradient, which extends above the mixing height.

For conditions of negligible synoptic scale mean vertical velocity, the equations governing the rate of growth of the convectively driven mixed layer are,

$$d\theta_{BL}/dt = (1/z_i)(\overline{w'\theta_o'} - \overline{w'\theta_i'}) \qquad (3\text{-}4)$$

$$d\Delta\theta_i/dt = \gamma_i dz_i/dt - d\theta_{BL}/dt$$

$$= -\gamma_i \overline{w'\theta_i'}/\Delta\theta_i - (\overline{w'\theta_o'} - \overline{w'\theta_i'})/z_i \qquad (3\text{-}5)$$

$$dz_i/dt = -\overline{w'\theta_i'}/\Delta\theta_i \qquad (3\text{-}6)$$

$$-\overline{w'\theta_i'} = c_4\overline{w'\theta_o'} + c_5 u_*^3\theta_o/gz_i \ . \qquad (3\text{-}7)$$

θ_{BL} is the mixed layer temperature, the subscripts o and i refer to values at the surface and the top of the mixed layer, $\Delta\theta_i$ is the temperature jump

at the top of the mixed layer ($\Delta\Theta_i > 0$) and γ_i is the lapse rate above the mixed layer. Laboratory and atmospheric measurements suggest $c_4 = 0.2$ and $c_5 = 5$. The numerical solution to the set of equations, employing a morning radiosonde and the shelter temperatures through the day, is discussed in detail by Tennekes and Driedonks (1981) and Wilczak and Phillips (1984). Driedonks (1982) discusses practical application of the above method for cases with convective and mechanical entrainment into the mixed layer.

Based on dimensional arguments, many researchers speculate that the mixing height during neutral conditions can be determined from,

$$z_i = c_6 u_* / f, \tag{3-8}$$

where f is the Coriolis parameter and c_6 is an empirical constant (typically 0.2 - 0.3). As discussed by Yu (1978) and Wetzel (1982), the correlation of estimates of z_i by (3-8) with values determined from the Wangara field data, range between 0.2 and 0.5, indicating no more than 20% of the variability of z_i is explained. When an inversion is present, z_i is given by the inversion base or (3-8), whichever yields the smallest value.

For nighttime stable conditions, we propose the mixing height be determined from (Zilitinkevich, 1972; Andre, 1983),

$$z_i = 0.4\ (u_* L/f)^{1/2}. \tag{3-9}$$

As stated before, the turbulent mixing depth may differ from the surface inversion depth during stable conditions. Several authors have worked on the evolution of the nocturnal surface inversion depth in combination with the temperature profile in the boundary layer (Yamada, 1979; Nieuwstadt 1980a; Stull, 1983a,b). At present, we suggest the inversion depth be estimated during stable conditions as suggested by Stull (1983a,b). This will be discussed in section 4.2.

4. PROFILES

4.1 Wind Profile

In the atmospheric surface layer the wind profile can be described successfully with Monin-Obukhov similarity theory (Yaglom, 1977). In the mixed layer and free convection layer during daytime, the wind speed and direction remain nearly uniform with height. For stable conditions, however, the wind speed increases with height often to a maximum, or low-level jet, near the top of the inversion layer.

A procedure is proposed for the derivation of the wind profile from a single observation of wind speed near the surface (10 m), an estimate of the roughness length z_o and the Obukhov length L. If estimates of geostrophic wind speed or free atmospheric wind speed are available, these can be employed as well.

For the mixed layer, we assume uniform distributions for wind speed. In the free convection and surface layer, the variation of the wind speed is given by,

$$U = U_r \frac{\ln(z/z_o - \Psi(z/L)}{\ln(z_r/z_o) - \Psi(z_r/L)}, \qquad (4\text{-}1)$$

where a general expression for Ψ is given by Paulson (1970) and z_r is the measurement height of the wind speed U_r.

For the near neutral upper layer, we assume U is given by (4-1). The change of wind direction is expected to be quite small during these neutral conditions, of the order of 10° over the first 200m. A procedure proposed

by Van Dop et al. (1982) could be employed to approximate the wind profile as,

$$U_z = f_s\ U + f_g\ G \cos D, \tag{4-2a}$$

$$V_z = f_g\ G \sin D, \tag{4-2b}$$

where U_z and V_z are the components of the wind speed, D is the angle between the surface wind direction and the direction of the Geostrophic wind and G is the Geostrophic wind speed. Note that we have chosen the x-axis along the surface wind direction. The precise characterization of the weighting functions (f_s and f_g) is of little concern so long as they are continuous, vary smoothly as a function of z/z_i between 0 and 1 with $f_s + f_g = 1$, and $f_s = 1$ for $z/z_i = 0$.

For stable conditions with $z/L < 0.5$, the wind speed can be estimated using (4-1) and (4-2). When $z/L > 0.5$, U can be better estimated using a semi-empirical extension of the log-linear profile given by Holtslag (1984a) as,

$$U = U_r \frac{\ln(z/z_o) + 7\ln\zeta + 4.25/\zeta - 0.5/\zeta^2 + 0.852}{\ln(z_r/z_o) + 5\zeta_r}, \tag{4-3}$$

where $\zeta = z/L$ and $\zeta_r = z_r/L$. With this profile it was shown that relatively good estimates can be obtained of the magnitude of U in very stable conditions up to z_i. A yet unresolved problem with the stable boundary layer is a description of the significant turning of wind with height. This turning can be 40° or more over the first 200m.

In the above, we have used values of G. For G we may use the surface geostrophic wind speed evaluated from surface pressure charts. Also, a free atmospheric wind or the 850 mb wind obtained from linear interpolation between

subsequent radiosondes may be used. Neither estimate of G is considered very accurate.

4.2 Temperature Profile

The potential temperature is constant within the mixed layer and the free convection layer (Tennekes and Driedonks, 1981). For heights greater than z_i, the temperature profile has to be obtained from radiosonde data. For heights below z_i, conditions are well mixed and the potential temperature is that recorded at the highest level of a tower or in the case when such measurements are not available at shelter height. This neglects the conditions that occur during strong heating, where a strong temperature gradient exists near the ground.

In the absence of strong heating or cooling at the surface or when the wind speeds are strong (6 m/s or more), day or night, the interpolated radiosonde temperature can be used with no modifications.

During the nighttime with strong radiational cooling or weak winds, the temperature profile and the inversion depth can be estimated using the procedures proposed by Stull (1983a,b). The nighttime sensible heat-flux history, together with the surface temperature decrease after sunset, are used to define the potential temperature profile as,

$$\Delta\theta/\Delta\theta_s = \exp(-az/H_I), \qquad (4\text{-}4)$$

where $\Delta\theta_s = \theta_s - \theta_o$

$\theta_s(t)$ = the surface potential temperature found at time t since transition,

θ_o = the potential temperature of the adiabatic profile at transition time,

$\Delta\Theta$ = $\Theta(t,z) - \Theta_o$,

$\Theta(t,z)$ = the potential temperature at height z at time t since transition,

H_I = $(1/\Delta\Theta_s) \int_{to}^{t} (\overline{w'\Theta'})\, d\tau$,

a = an empirical constant found to be about 0.77 by Stull for the Wangara and Koorin experiments (nearly uninhabited sites that were relatively dry).

The time of transition t_o is defined as that instant when the net sensible heat flux at the surface changes sign from positive to negative. Stull(1983b) demonstrates using Wangara field data that h is well estimated as $5H_I$. For large-scale advection effects, the surface temperature θ_s could be increased (decreased) to account for increases (decreases) of the 700 mb temperatures between successive radiosondes. Such a procedure was employed successfully by Benkley and Schulman (1979) and Garrett (1981) to adjust for large-scale advection effects in their estimates of the growth of the unstable boundary layer.

4.3 Turbulence Profiles

In the mixed layer, Caughey (1982) notes that the observations of the rms variance of the vertical velocity σ_w suggest a broad maximum centered at $z_i/2$ where σ_w^2 is $0.4w_*^2$. The numerical simulations of the convective boundary layer by Deardorff (1974) suggest the height of maximum variance is $z_i/3$. Caughey (1982) reports that near z_i, water tank and numerical results indicate σ_w^2 is $0.1w_*^2$ in agreement with the 1976 Ashchurch field data. Above z_i, Caughey reports that σ_w^2 decreases to $0.01w_*^2$ near $1.5z_i$.

During the nighttime, when the atmosphere is stratified, the vertical wind-speed fluctuations in theory decrease in amplitude as a function of

height, to near-zero values at z_i (Caughey, 1982 and Yamada, 1979). A reasonable fit to the 1973 Minnesota stable field data is,

$$\sigma_w^2/u_*^2 = A_w(1 - z/z_i)^d, \qquad (4\text{-}5)$$

where σ_w is the standard deviation of the vertical wind-speed fluctuations, $A_w = 2.2$ and $d = 3/2$. Nieuwstadt (1983) using data collected from the 213 m meteorological tower at Cabauw found $A_w = 1.7$ and $d = 3/2$. The significance of Nieuwstadt's results is that he arrived at (4-5) using local scaling arguments. Measurements of σ_w^2 may be considerably influenced by gravity wave contributions. For that reason, Nieuwstadt employed high pass filtered data for the determination of A_w and d.

The standard deviation of the cross wind-speed fluctuations, σ_v, in the surface layer is poorly characterized using Monin-Obukhov similarity scaling, especially within the stable surface layer, see Panofsky et al. (1977). During convective conditions, the numerical simulations of the convective boundary layer and the atmospheric data suggest a slight maximum near $0.8z_i$ in σ_v; the average value over the entire profile for σ_v^2 is $0.4w_*^2$.

During stable conditions the mean wind direction show sizeable intermittent sudden changes (meandering). This phenomenon may result from various factors such as the slope of the terrain, location of hills in the upwind fetch and movement of weather systems. Although meander is most often observed during very stable conditions, this does not preclude its occurence during other times. Strong mixing during unstable conditions might mask the contributions due to meander to σ_v but the contributions to the energy spectra are

still present. Højstrup (1981, 1982) and Berkowicz and Prahm (1982) found success in modeling the velocity spectra as consisting of a buoyancy-produced part and a shear-produced part. The modeled variances by Højstrup (1982) agree well with data from the Kansas and Minnesota field experiments. His results for the w-spectra are valid only for the lower half of the boundary layer, where the long-wavelength fluctuations can be assumed to be damped by the presence of a solid lower boundary mechanically impeding the vertical fluctuations. As a working hypothesis for modeling the vertical velocity variance, we could combine the shear-produced variance, as modeled by Højstrup (1982), with the buoyancy-produced variance, as modeled by Baerentsen and Berkowicz (1984). The resulting characterizations of the lateral and vertical variances would be,

$$(\sigma v/u_*)^2 = \begin{cases} 0.7(z_i/L)^{2/3} + \dfrac{2.7(1-z/z_i)^2}{(1+2.8z/z_i)^{2/3}} & \text{for } L < 0 \\ 2.7\,\dfrac{(1-z/z_i)^2}{(1+2.8z/z_i)^{2/3}} & \text{for } L \geq 0 \end{cases} \qquad (4\text{-}6)$$

$$(\sigma_w/u_*)^2 = \begin{cases} 1.54[z/(-kL]^{2/3}\exp(-2z/z_i) + 1.457(1-z/z_i)^2 & \text{for } L < 0 \\ 1.457(1-z/z_i)^2 & \text{for } L \geq 0 \end{cases} \qquad (4\text{-}7)$$

The expression (4-7) fits quite well the 1973 Minnesota field data for unstable conditions .

The estimate of the lateral variance neglects meander. The linear decrease of σ_w with height, while appropriate during daytime neutral conditions, would not reflect the height dependence observed during stable conditions. This deficiency although noticeable in the mean under ideal

conditions would likely not be noticeable in practice, owing to the variations caused by conditions differing from ideal. Recently, the low frequency part of the spectra of the velocity components under stable conditions has been successfully modeled by Larsen et al. (1983). The low frequency part of the horizontal velocity components were found to be fairly well described by a $N^2\kappa^{-3}$ law, where N is the Brunt-Väisälä frequency and κ the horizontal wave number.

5.0 DIFFUSION

The applicability of employing scaling parameters for describing the turbulence in the air depends on the extent to which the actual circumstances approach the idealized conditions specified in the basic theoretical and experimental studies. Reliable specification of the turbulence and thereby the diffusion cannot be expected if the airflow is uncertain or calm, or if the airflow has been complicated by local circulations induced by heating or cooling or hilly terrain. Little success can be expected in the immediate vicinity of buildings and obstacles. The methods described here for diffusion estimates do not account for effects of deposition or reactions in the atmosphere, and are only valid for distances less than 10 km.

Even when the actual conditions approach the ideal conditions, the practical problems of estimating the expected distribution of concentration are significant. The comparison results summarized in Pasquill's (1974) Table 6.XI suggest that even under ideal circumstances 20 to 30% deviations from the mean concentration values can be expected for ensemble average estimates for particular meteorological conditions. For individual comparisons deviations of about 50% appear likely (Gryning and Lyck, 1984).

This chapter summarizes some of the relationships of the basic scaling parameters to diffusion processes. A description of the pollutant distribution necessarily includes (implicitly or explicitly) the shape of the distribution, the dimensions of the diffusing cloud, and the boundary conditions. The shape describes the vertical and horizontal profiles of the cloud. The dimensions are often specified by the root mean squared deviations σ_y and σ_z of the pollutant mass along the coordinate axes. The values σ_y and σ_z are

typically referred to as the dispersion parameters. Often they are associated with a Gaussian shaped distribution but, of course, this is not necessary.

A traditional basis for describing diffusion is the Taylor diffusion theory which relates the mean square particle displacement, σ_y^2, to the cross wind velocity variance, σ_v^2, through,

$$\sigma_y^2 = 2\ \sigma_v^2 \int_0^t \int_0^T R(\xi)\ d\xi dT, \tag{5-1}$$

where t is travel time and R (ξ) the Lagrangian autocorrelation function and,

$$\lim_{T \to \infty} \int_0^T R(\xi)\ d\xi = T_L,$$

the Lagrangian integral time scale. In the limit (5-1) becomes,

$$\sigma_y = \sigma_v\ t \qquad \text{for small t;} \tag{5-2}$$

$$\sigma_y = \sigma_v (2T_L)^{1/2}\ t^{1/2} \qquad \text{for large t.} \tag{5-3}$$

These relationships were derived for an ensemble average of particle displacements during conditions of stationarity and homogeneity. Pasquill (1971) derived from Taylor's theory the following expression for estimating the lateral diffusion,

$$\sigma_y = \sigma_v\ t\ f_y, \tag{5-4}$$

where f_y is a universal function (of transport time and a time scale) that describes the growth of the dispersion parameters during transport downwind. The standard deviation of wind fluctuations, σ_v, is to be computed for the interval over which the concentrations values are averaged. Gryning (1981) and Gryning and Lyck (1984) argue the f_y depends on atmospheric stability, release height, downwind distance and wind velocity. Often, the downwind distance and wind velocity are combined into a travel time (Draxler, 1976).

Sivertsen (1978) argues that f_y responds to the overall structure of the turbulence; whereas, σ_v describe the local features of the terrain.

A comparison was performed of five empirical forms suggested for f_y (Irwin, 1983) with field tracer data collected at 11 sites. Draxler's (1976) scheme performed best, a finding which is in agreement with Gryning and Lyck (1984). Irwin (1983) noted that selecting a simple expression for f_y that is invariant with height resulted in little overall loss in performance. We recommend,

$$f_y = 1/[1 + 0.9\ (t/T_e)^{1/2}], \tag{5-5}$$

where T_e = 1000 s.

If we view the total diffusion as the summation of individual effects of each process [Högström (1964) and Pasquill (1976)], then,

$$\sigma_y^2 = \sigma_{yo}^2 + \sigma_{yb}^2 + \sigma_{ys}^2, \tag{5-6}$$

where σ_{yo} is estimated using (5-4) and (5-5), σ_{yb} is the induced diffusion due to buoyant plume rise effects, and σ_{ys} is the induced diffusion due to wind direction shear in the vertical. At this time, the magnitude of the buoyancy effects on the lateral diffusion is uncertain. It seems σ_{yo} dominates initially with σ_{ys} becoming of increasing importance at large downstream travel time. Pasquill and Smith (1983) investigated the effect of wind shear on the horizontal diffusion and found the distance of travel at which the effect of σ_{ys} becomes important. They conclude that the effect is not important within about 5 km from an elevated source or within about 12 km of a ground-level source.

In the following, expressions are provided for characterizing the dispersion for each of the regimes described in Chapter 2. In some cases, expressions are given for estimating the crosswind integrated concentration,

$$\chi^y(x) = \int_{-\infty}^{\infty} \chi(x,y)\, dy$$

where χ (x,y) is the surface concentration. The x-coordinate axis is aligned along the surface wind direction. Given χ^y we can compute χ assuming a Gaussian distribution of the material in the crosswind as,

$$\chi(x,y) = \frac{\chi^y(x)}{\sqrt{2\pi}\ \sigma_y} \cdot \exp(-y^2/2\sigma_y^2). \qquad (5\text{-}7)$$

Even though the vertical distribution of material may be other than Gaussian, the lateral distribution is well approximated using (5-7), as discussed by Deardorff and Willis (1975), Gryning and Lyck (1980) and Gryning et al., (1978).

In general, the total vertical diffusion is a combination of turbulent diffusion and the effects of buoyant plume rise, σ_{zb}, as

$$\sigma_z^2 = \sigma_{zo}^2 + \sigma_{zb}^2. \qquad (5\text{-}8)$$

For elevated sources well above the surface and below the inversion, a similar approach for estimating σ_{zo} as shown above for σ_y, (5-4), could be applied when σ_w is available. Field data suggest that σ_{zb} scales with plum e rise (Briggs, 1975).

In the following, examples are given demonstrating the relationship of the basic meteorological parameters to the description of vertical diffusion for each of the regimes described in Chapter 2.

5.1 The Surface Layer (unstable and stable conditions)

A number of investigations have demonstrated the applicability of Monin-Obukhov similarity theory to describing the diffusion of near surface releases by use of K models, (Nieuwstadt and Van Ulden, 1978, Gryning et al., 1983, Sivertsen et al., 1983).

Within the surface layer, the vertical eddy diffusivity of matter, K, can be expressed generally as,

$$K = ku_{\star}z/\phi_h(z/L), \tag{5-9}$$

where $\phi_h(z/L)$ is an empirical function that describes the dependency on atmospheric stability, Table 5-1. When the wind and K profiles are represented by power laws, a general solution of the two-dimensional diffusion equation can be written as (Van Ulden, 1978),

$$\chi^y(z)/Q = (A/\overline{zu}) \exp\,[-(Bz/\overline{z})^s] \tag{5-10}$$

$$A = s\,\Gamma(2/s)/[\,\Gamma(1/s)\,]^2 \tag{5-11}$$

$$B = \Gamma(2/s)/\,\Gamma(1/s), \tag{5-12}$$

where Γ is the gamma function. The following equations are suggested for specifying the shape parameter s (Gryning et al., 1983) and the mean height of particles $\overline{z}$ (Van Ulden, 1978).

For $L > 0$:

$$s = \frac{1 + 2\,b_1\,c\overline{z}/L}{1 + b_1\,c\overline{z}/L} + \frac{1 + b_2\,c\overline{z}/L}{\ln(c\overline{z}/z_o) + b_2\,c\overline{z}/L}\,, \tag{5-13a}$$

$$x + x_o = (\overline{z}d/k^2)\,[\{\ln(c\overline{z}/z_o) + 2\,b_2p\overline{z}/(3L)\}\,[1 + b_1p\overline{z}/(2L)] + (b_1/4 - b_2/6)p\overline{z}/L)]. \tag{5-13b}$$

For $L < 0$:

$$s = \frac{1 - a_1\,c\overline{z}/(2L)}{1 - a_1\,c\overline{z}/L} + \frac{(1 - a_2c\overline{z}/L\,)^{-1/4}}{\ln(\,c\overline{z}/z_o) - \Psi(c\overline{z}/L)}\,, \tag{5-14a}$$

$$x + x_o = (\overline{z}d/k^2)\,[\,\ln\,(c\overline{z}/z_o) - \Psi\,(c\overline{z}/L)\,]\,[1 - p\,a_1\,\overline{z}/(4L)]^{-1/2}. \tag{5-14b}$$

x_o is an integration constant and is determined with $x = 0$ and $\overline{z}$ equal to the release height z_s.

For stable conditions ($L > 0$), we solve for the crosswind integrated concentration by first determining $\overline{z}$ (iteratively from 5-13b) for the given

distance downwind. With $\bar{z}$, we can solve for A and B for use in 5-10. A similar approach is followed for unstable conditions ($L < 0$).

Dyer(1974) proposed $a_1 = a_2 = 16$; $b_1 = b_2 = 5$ with $k = 0.41$. These coefficients were used by Gryning et al. (1983) and Holtslag (1984b). In the original derivation, Van Ulden (1978), used the coefficients proposed by Businger et al., 1971). In Table 5-1, the ϕ_m and ϕ_h functions are given together with the expression for the mean wind speed, $\bar{u}$, over the plume. The coefficients p and c are in fact dependent on s. For practical applications we propose $p = 1.55$ (Van Ulden, 1978) and $c = 0.6$ (Gryning et al., 1983).

TABLE 5-1. THE ϕ_h, ϕ_m AND $\bar{u}$ FUNCTIONS NEEDED FOR THE APPLICATION OF EQUATIONS (5-9) THROUGH (5-14).

For $L < 0$:

$$\phi_h(z/L) = d(1 - a_1\, z/L)^{-1/2}$$

$$\phi_m(z/L) = (1 - a_2\, z/L)^{-1/4}$$

$$\Psi(z/L) = 2\ln\{(1 + x)/2\} + \ln\{(1 + x^2)/2\} - 2\tan^{-1}(x) + \pi/2,$$

where $x = (1/\phi_m)$,

$$k\bar{u}/u_* = \ln(c\bar{z}/z_o) - \Psi(c\bar{z}/L).$$

For $L > 0$:

$$\phi_h(z/L) = d(1 + b_1\, z/L),$$

$$\phi_m(z/L) = 1 + b_2\, z/L,$$

$$k\bar{u}/u_* = \ln(c\bar{z}/z_o) + b_2\, \bar{z}/L\ .$$

Elliott (1961) found the shape parameter ranged from s = 1.0 from unstable conditions to about s = 2.0 for stable conditions. For a Gaussian concentration distribution s = 2, hence under unstable and neutral conditions a Gaussian concentration profile does not fit the observed vertical distribution.

5.2 The Mixed Layer

The mixed layer scaling is appropriate when $z_s/z_i > 0.1$ and $z_s/-L > 1$, where z_s is the release height. Deardorff and Willis (1975), Willis and Deardorff (1978), Lamb (1978, 1979) reported the results of a series of laboratory and numerical simulations of dispersion of nonbuoyant material in a well developed mixed layer. Deardorff and Willis presented tabulations of the dimensionless mean crosswind integrated concentration values at various heights and distances from the release at z_s/z_i of 0.067.

As an extension of these results, Briggs (1985) reanalyzed the dimensionless cross-wind integrations both from the laboratory and the numerical simulations. It was found that the mean cross-wind integrated concentration results at the surface could be well characterized as,

$$\chi^{y}z_i \, U/Q = \frac{0.9 \, X^{9/2} \, Z_s^{-11/2}}{[Z_s^{-3/4} + 0.4 \, X^{9/2} \, Z_s^{-9/2}]^{4/3}} + \frac{1}{[1 + 3 \, X^{-3/2} \, Z_s^{1/2} + 50 \, X^{-9/2}]} , \qquad (5\text{-}15)$$

where $X = (x/z_i)(w_*/U)$ and $Z_s = z_s/z_i$. This expression applies for nonbuoyant releases when $1 \geq Z_s \geq 0.04$.

Recently, Willis and Deardorff (1983) reported the findings of a series of laboratory simulations of buoyant releases within a well developed convective boundary layer. They found that plume buoyancy effects became

noticeable in the diffusion results where the plume buoyancy parameter $F^* = F/(Uw_*^2 z_i)$, exceeded about 0.02, where F is the standard definition of plume buoyancy. The vertical distribution of concentration within the plume was highly skewed and non-Gaussian. Tabulations of χ^y are not available for a wide variety of values of F* and a suitable number of release heights for a recharacterization of (5-15) including buoyant plume rise effects.

5.3 The Free Convection Layer

Free convection exists in the layer above z = -L and and below $z \sim 0.1 z_i$ where z, u_f and θ_f are the controlling parameters. Nieuwstadt (1980b) analyzed the portion of the Prairie Grass data measured under convectively unstable conditions and found that free convection similarity scaling was appropriate for those cases downwind when $0.03 < X < 0.23$. The normalized crosswind integrated concentration is then given by,

$$\chi^y z_i U/Q = bX^{-3/2} \qquad (5\text{-}16)$$

where b is 0.9. Holtslag (1984b) compared the surface similarity predictions by (5-10) versus the free convection predictions by (5-15) using the Prairie Grass data. At x = 50 m it was seen that the surface layer model performed better than the free convection model, comfirming that at x = 50 m the plume was still within the surface layer. At x = 200 m and 800 m the surface layer model and the free convection model predictions were similar. This would suggest that both scaling principles can be applied to these distances. Deposition was not considered in the analyses by Nieuwstadt (1980b) and Holtslag (1984b). Gryning et al. (1983) show that consideration of deposition significantly improves the predictions of the surface layer model, especially at x = 800 m.

5.4 The Entrainment Layer

For unstable conditions, the entrainment layer extends between $z > 0.8z_i$ and $z < 1.2z_i$. For strongly buoyant releases, the possibility exists for material to become stabilized in the layer above z_i. The amount of material which "penetrates" into the stable layer capping the mixed layer is dependent on (Briggs, 1975),

$$p_s = F/(U\gamma_i z_i'^3) \tag{5-17}$$

where $z_i' = z_i - z_s$ and γ_i = the potential temperature gradient in the capping inversion. The fraction of material, P, that stabilizes in the capping inversion is estimated by Weil and Brower (1982) as,

$$P = 1.5 - (1/2.6)/p_s^{1/3}. \tag{5-18}$$

This penetration estimate suggests that full penetration occurs when $p_s > 0.44$. Penetration of 50 % is estimated when $p_s = 0.129$. These estimates suggest that it requires only 13% as much buoyancy to achieve 50% penetration as that required to penetrate fully. Laboratory simulations for a strongly buoyant effluent ($F^* > 0.1$) with a strong capping density jump ($p_s < 0.05$), suggest that the plume tends to loft against the capping inversion (Willis and Deardorff, 1983). It appears that the plume still retains sufficient buoyancy to resist mixing down towards the surface.

5.5 Near Neutral Upper Layer

Knowledge of the diffusion in the near neutral upper layer is very limited. For releases in the near neutral upper layer we therefore recommend the use of the traditional Gaussian plume model for estimating concentrations.

Measurement of σ_w and σ_v are preferred for use with (5-4) and (5-5) to estimate the lateral and vertical dispersion parameters for use in the Gaussian model. Otherwise, σ_w and σ_v can be approximated using (4-6) and (4-7). For f_z the value of T_e is recommended to be 500s (Draxler, 1976; Irwin, 1983).

5.6 Local Scaling Region

For characterizing the diffusion in this region we recommend the use of the Gaussian plume model for estimating concentrations. Measurements of σ w and σ_v are preferred for use in (5-4) and (5-5) to estimate the lateral and vertical dispersion parameters, although measurements may be strongly influenced by waves. An example of atmospheric diffusion under stable conditions that is completely dominated by waves is given in Gryning et al. (1985). Otherwise, σ_w and σ_v can be approximated using (4-6) and (4-7). For f_z the value of T_e is of the order 50 s (Irwin, 1983). The difficulty in the use of (4-6) and (4-7) is that the turbulence fluctuations, and hence σ_w and σ_v, scale on local values of u_* and Λ.

Recently, Venkatram et al. (1983) reported findings from experiments conducted at Cinder Cone Butte, demonstrating that the vertical diffusion parameter could be well estimated using (5-4) with,

$$f_z = (1 + t/2T_L)^{-1/2}, \tag{5-19}$$

where T_L = the Lagrangian time scale, estimated as ℓ/σ_w,

ℓ = the length scale, estimated as, $(1/\ell_s + 1/\ell_n)^{-1}$ where ℓ_s is the stable length scale and ℓ_n is the neutral length scale,

$\ell_s = \gamma^2 \sigma_w/N$, where $\gamma = 0.522$,

$\ell_n = \alpha z$, where $\alpha = 0.36$,

N = the local value at z of the Brunt-Väisälä frequency, $[(g/T)(\partial\theta/\partial z)]^{1/2}$,

σ_w = the local value at z of the standard deviation of the vertical velocity fluctuations.

Substituting typical values into (5-19) and solving for T_L, shows T_L is approximately 8 to 12 s. The expressions (5-5) and (5-19) for f_z are nearly equivalent when $T_e = 4.86T_L$. Hence, these results reported by Venkatram et al. (1983) are in accord with the findings reported by Irwin (1983) for T_e = 50 s for stable conditions. The information provided by Venkatram et al. (1983) shows that local z-less scaling arguments can be employed to describe the diffusion processes.

6.0 DISCUSSION

An outline of methods for processing meteorological data for use in diffusion modeling has been presented. To incorporate the proper scaling parameters the discussion was structured in accordance with current concepts for the idealized states (regimes) of the planetary boundary layer. The goal was to characterize the meteorological conditions affecting the diffusion for transport distances on the order of 10 km or less. The distance to the maximum ground-level concentration is often within this range.

The diffusion is routinely found to be other than Gaussian in the vertical (Gryning and Lyck, 1984). Therefore, whenever justified we have recommended the use of techniques that characterize directly the crosswind integrated concentrations at the surface. For elevated releases within the near neutral upper layer and the stable (local scaling region) we recommend use of the Gaussian plume model, where the dispersion parameters are estimated using statistical methods. Little is known regarding diffusion within the entrainment layer.

A special complication in the use of the suggested methods arises when the proper state of the diffusion process is at the border line between two regimes. Such cases will give rise to a jump in concentration dependent on the choice. No procedures have been devised to avoid these jumps in calculated concentration.

For obtaining the meteorological data needed for estimating the fundamental meteorological scaling parameters, we recommend as a minimum a measurement program as presented in Table 6-1. The measurements should be carried out at a mast. The upper measurement level should be at a height $100z_o$, but not less than 10m. The lower measuring level should be at $20z_o$, but not less than 1m. Here, z_o is the effective surface roughness length and can be estimated from Table 3.1. Also discussed in this report are methods for determining the fundamental scaling parameters if only synoptic meteorological data are available.

We anticipate that the suggested characterizations of the diurnal variation of the wind speed and direction profiles are too simplistic and will need further development. Furthermore, the turbulence profiles are highly idealized as the assumption is made that above the mixed layer the turbulence is negligible. To complete the development of a meteorological processor, the methods outlined should be tested using available data. With the test results, future research can focus on those estimation methods requiring the greatest improvement and on developing methods to characterize the spatial variations in the meteorological variables.

TABLE 6-1. RECOMMENDED MINIMUM MEASUREMENT PROGRAM
THE TYPICAL SAMPLING DURATION SHOULD BE 10 MINUTES.

PARAMETER	SAMPLING RATE (sec)	MEASURING HEIGHT	EXAMPLE INSTRUMENTS**
Wind speed	1 to 5	Upper level	Cup anemometer
Wind direction	1 to 5	Upper level	Wind vane
Longitudinal Turbulence	*	Upper level	Cup anemometer
Wind direction fluctuation	*	Upper level	Wind vane
Temperature	10	Upper level	Resistance
Temperature difference	10	Upper level to lower level	Fast Thermocouples

* Estimated from wind speed and direction measurements.

** Instruments should be well designed for the purpose. Minimum instrument requirements are given in Hoffnagle et al. (1981) Table 1.

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